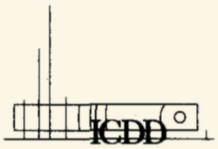
Powder Diffraction



Volume 6 Number 1 March 1991
Powder Diffraction An international journal of materials characterization

SIEMENS

Ask for performance - ask for the new D 5000 x-ray diffractometer

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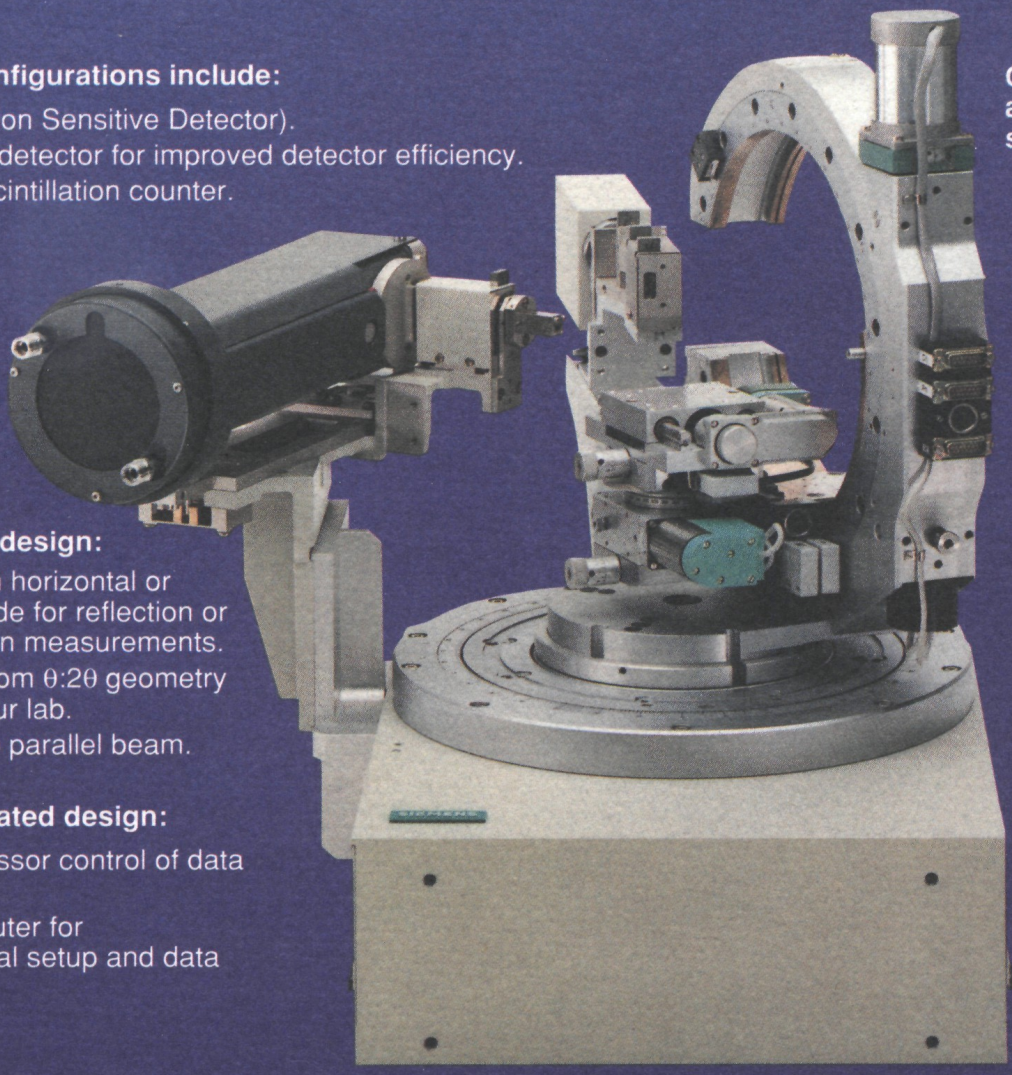
- PSD (Position Sensitive Detector).
- Solid-state detector for improved detector efficiency.
- Standard scintillation counter.



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- Operates in horizontal or vertical mode for reflection or transmission measurements.
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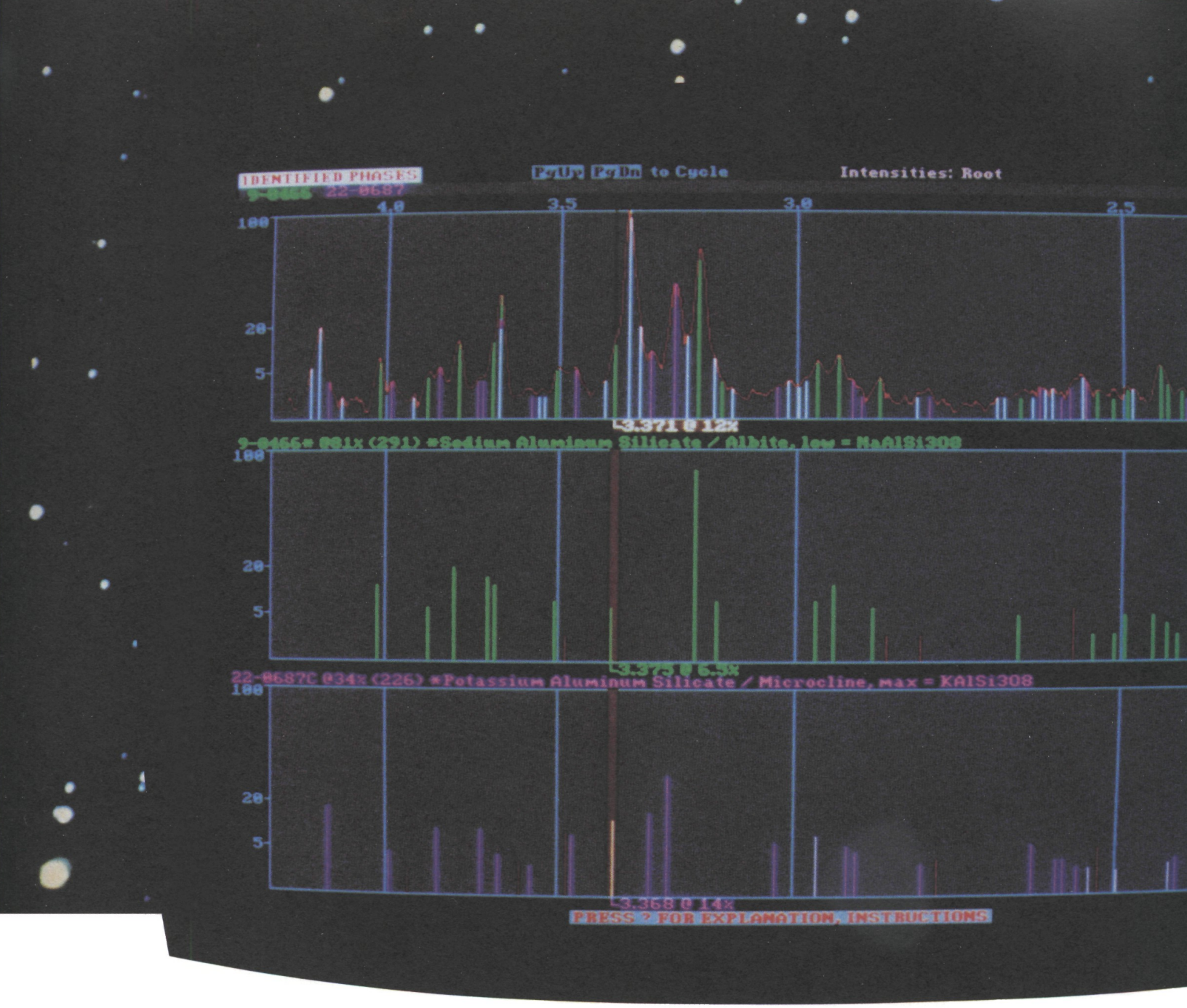

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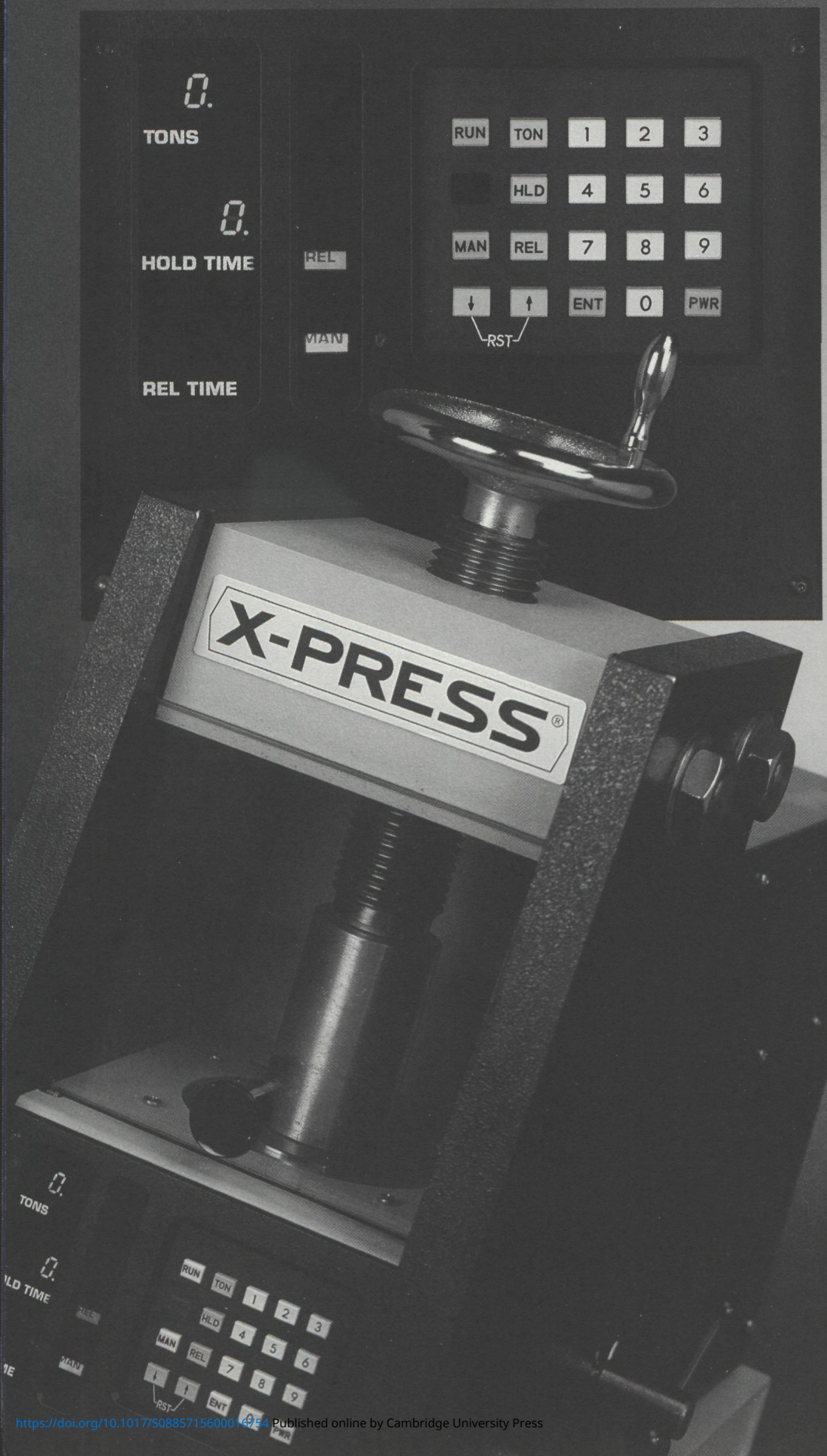

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Powder Diffraction

An International Journal of Materials Characterization

Publisher
JCPDS-International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, Pennsylvania 19081, U.S.A.

Powder Diffraction is a journal of practical technique, publishing articles relating to the widest range of application – from mineral analysis to epitactic growth of thin films and to the latest advances in software. Although practice will be emphasized, theory will not be neglected, especially as its discussion will relate to better understanding of technique.

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Subscriptions. The annual subscription rate in the United States and Canada is $45.00; Library; $85.00; other than U.S.A., Canada and the Far East, the annual subscription is $65.00. Subscriptions to the Far East, including Japan, China, Taiwan, Malaysia, the Philippines, Indonesia and Korea should be made via Sanyo Information System Corp., Taiyo Bldg. 7-7, Tomizawa-cho Nihonbashi, Chuo-ku, Tokyo 103, Japan. Airmail delivery available for subscribers outside U.S./Canada for an additional cost of $35.00 per volume (4 issues).

Payment may be made in U.S. dollars by company check, MasterCard, Visa or international money order. Please address communications to the publisher's office.

Advertising. For advertising rates and schedules contact the Publisher's Office JCPDS-International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19082, Telephone (215) 328-9405.

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Postal Information. Powder Diffraction (ISSN 0885-7156) is published quarterly for $45.00 a year (U.S. and Canada) by JCPDS-International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, Pennsylvania 19081. JCPDS principal office: 1601 Park Lane, Swarthmore, Pa. 19081. Julian Messick, Jr., General Manager.

Postmaster: Send address changes to JCPDS-International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, Pennsylvania 19081.

International CODEN Service (Intercode): PODIE2
ISSN 0885-7156
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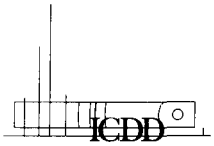

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APD 2000
Diffractometric System

GD 2000 Goniometer

- High resolution
- 2 step motors
- Horizontal and vertical configuration

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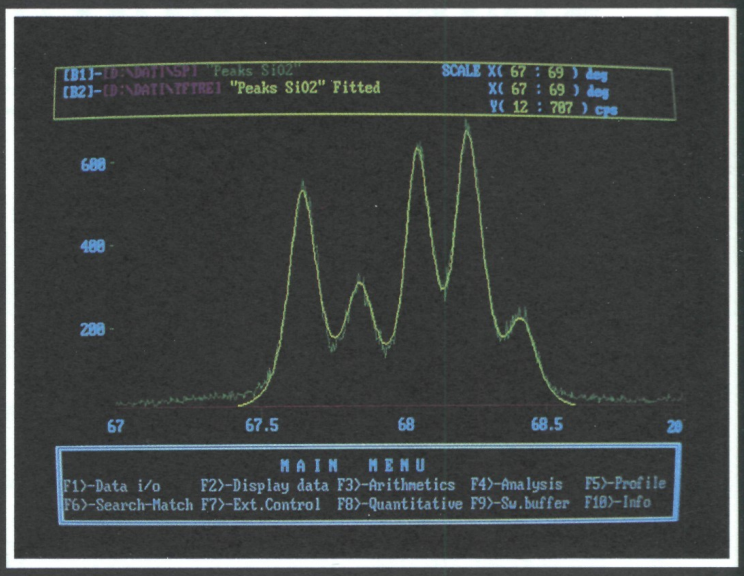
Seeman-Bohlin geometry



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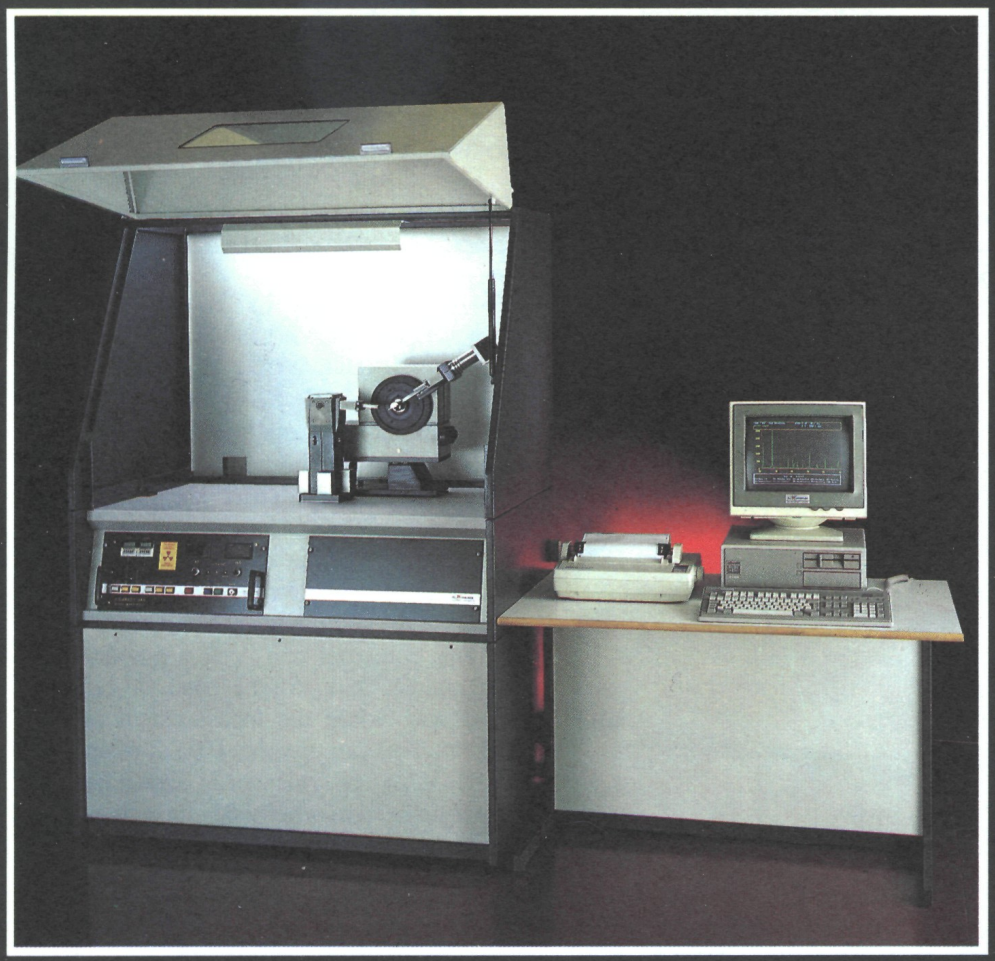

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- Search-Match
- Crystallinity
- Quantitative Analysis
- Stress

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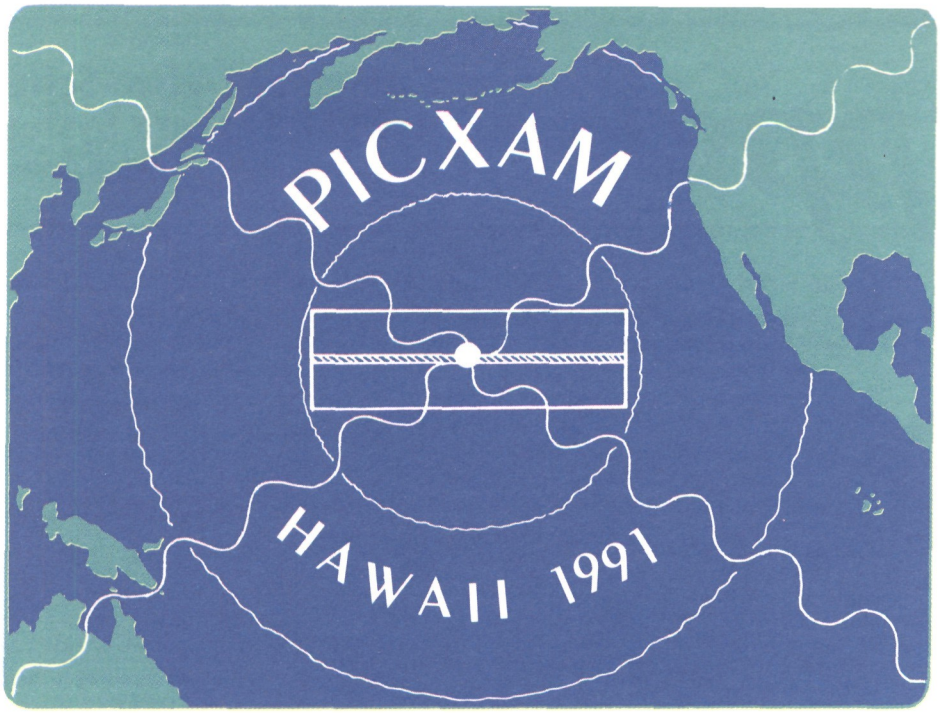

Second Announcement...

The first international congress on X-ray Analytical Methods for Materials Analysis will be held in Honolulu, August 12-16, 1991, at the Hilton Hawaiian Village.

Congress Theme...

The major thrust of this meeting will be related to the practical aspects involved in X-ray methods for materials analysis. This will be in keeping with the tradition of the Australian X-Ray Analytical Association (AXAA), the Denver X-Ray Conference and the X-Ray Chemical Analysis Group of the Japan Society of Analytical Chemistry.

To be discussed will be the use of X-ray methods based on Powder Diffraction, Fluorescence, Surface Analysis, Absorptiometry, Column Electron Diffraction and Thin Film Characterization by X-ray Diffraction, and Trace Analysis and Thin Film Characterization by X-Ray Fluorescence.

A two day pre-congress workshop program will be held at the University of Hawaii at Hilo, on August 8 and 9.

PICXAM is organized by:

The Australian X-ray Analytical Association
The Denver X-ray Conference
X-ray Chemical Analysis Group/
Japan Society for Analytical Chemistry

PICXAM is cosponsored by:

The International Centre for Diffraction Data
The University of Denver
The University of Hawaii

PICXAM

Pacific-International Congress on X-Ray Analytical Methods

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PC-PDF

The Powder Diffraction File on CD-ROM

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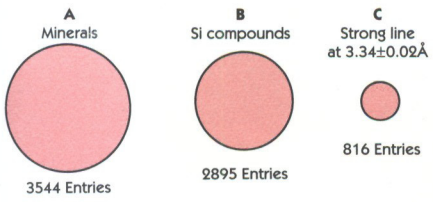
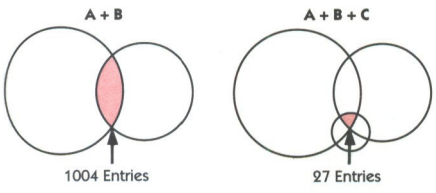
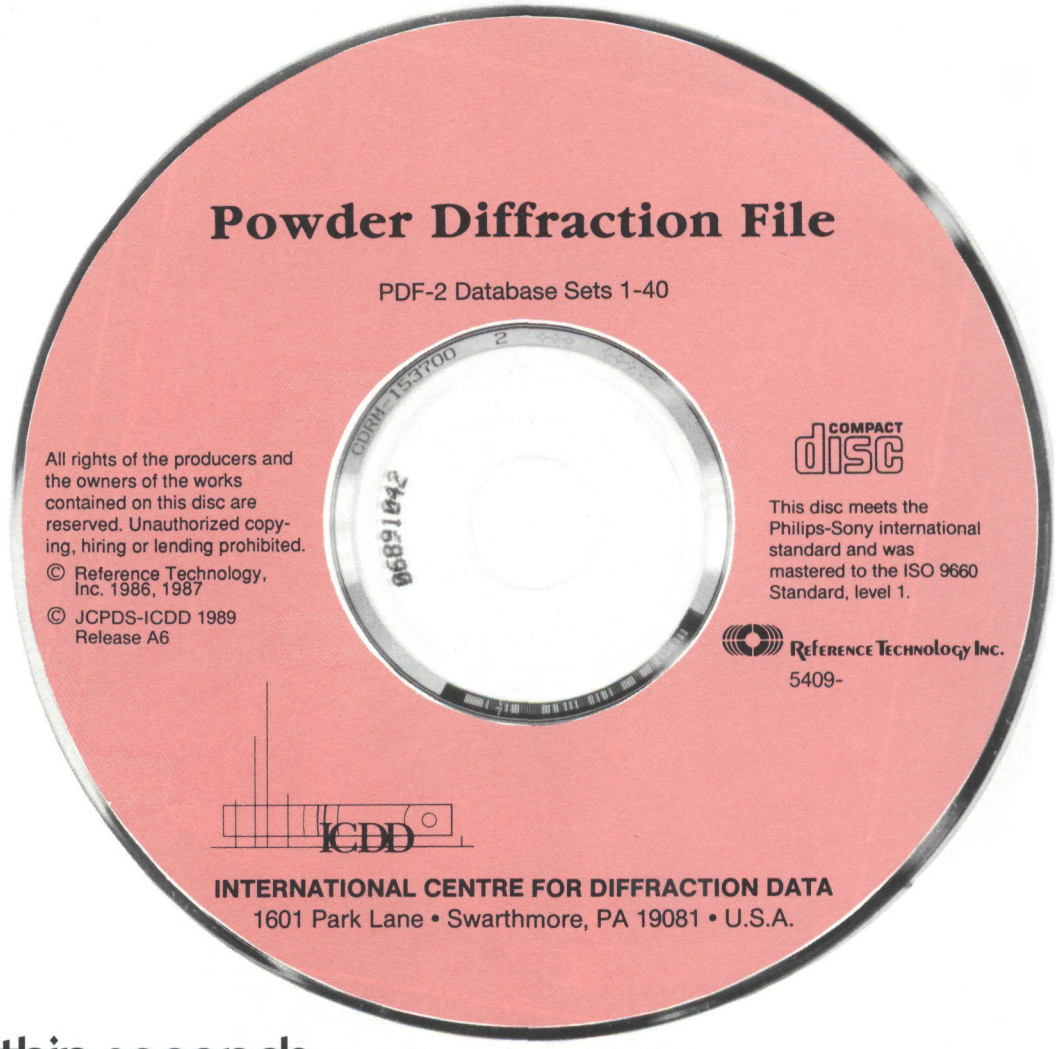


Search on combinations of fields.





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Editorial

Calculated Powder Patterns are a Welcome Addition to New Diffraction Data Articles

In this journal a calculated powder pattern is a welcome addition to an article incorporating new diffraction data. The calculated pattern tells the reader how well an observed diffraction pattern agrees with a theoretical pattern based on the crystal structure of the compound and the techniques employed to measure the pattern. We urge authors who submit new powder diffraction data, and who also have access to single crystal structure data on the compound, to provide an additional column of calculated intensities in their data tables.

A calculated pattern is an invaluable indexing aid for large volume, lower symmetry unit cells where, based on calculated ds alone, there can be numerous possible hk*l*s to account for each experimental peak. Based on calculated intensities, the more intense reflection(s) contributing to the peaks is (are) selected for the unit cell parameter refinement. The result is almost always improved precision and accuracy. Including the calculated intensities of reported reflections validates the indexing.

If intensity agreement between observed and calculated patterns is poor, unsupected preferred orientation in a diffractometer specimen can be recognized.

A calculated pattern of a newly synthesized compound prepared with the new compound's scattering factors, but using the atomic positions of an isostructural compound, can be an important "proof of structure type" if there is good agreement between calculated and observed patterns.

Like an experimental powder pattern, the calculated powder pattern also requires a certain amount of documentation. The editors request that the following information be provided when a calculated pattern is included in a manuscript:

- Source of atomic position data. Note any partial occupancy used to model defects, or fractional occupancy used to model solid solution.
- Scattering factors used. Note whether these were neutral or ionized and whether anomalous dispersion was included.
- Thermal parameters and their source. Note whether these were isotropic or anisotropic, whether none were employed, or whether thermal parameters were estimated (*e.g.* all atoms assigned (B iso) = 1.00).
- Note options chosen to model the experiment, *e.g.* incident or diffracted beam monochromator polarization corrections; theta- compensating variable divergence slit, etc.
- State whether integrated or peak relative intensities are tabulated. If peak, document the profile function and the instrumental and sample broadening used in the powder pattern simulation. Note whether or not the peak intensity profile includes both α_1 and α_2 components of the α doublet.

Most powder pattern calculation codes provide only integrated relative intensities which are not fully comparable to observed peak intensities. However, integrated intensities can still be useful for validating indexing and identifying preferred orientation. One must clearly label these as integrated intensities in data tables. We recommend including 2θ, d and integrated relative intensity of all reflections with $I > 0.5$.

Even with codes that provide relative intensities, a quantitative comparison of observed and calculated intensities is far from routine. One must ensure that the profile imposed on the integrated intensities properly models both the instrument and the sample induced broadening of peaks, whether inclusion of the alpha doublet is or is not appropriate, and when a peak is considered "resolved".

When a calculated pattern which closely models the data collection conditions is available, it is desirable to have a quantitative measure of the agreement between observed and calculated intensities. In this issue, Charlotte Lowe-Ma suggests an intensity figure-of-merit based on the average percent difference between observed and calculated intensities (integrated in her case) for a limited number of strong and moderately-strong peaks. While recognizing that this figure-of-merit has its limitations, especially where overlap of strong reflections is common, we recommend its use as a means of describing the extent of agreement between the stronger observed and calculated intensities important to phase identification. We look forward to additional proposals for intensity figures-of-merit.

Finally, as this writer, and anyone else who regularly calculates powder patterns, knows, errors can confound the unwary. A single mistyped site multiplicity or atomic position can easily lead to an erroneous calculated pattern that gives little sign of being in error. Often, it is disagreement of relative intensities with those of an observed pattern that leads one to return to a careful proofreading of the input data or even to a mistake made in the original crystal structure publication or database entry based on it. Authors are urged to be especially cautious with their powder pattern calculations, and to use all available means (interatomic distance calculations, density checks, etc.) to validate their results.

G. J. McCarthy
Editor for New Diffraction Data